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Explosive Model Tarantula V1/JWL++ Calibration of LX-17: #2

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Explosive Model Tarantula V1/JWL++ Calibration of LX-17: #2

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Abstract: Tarantula V1 is a kinetic package for reactive flow codes that seeks to describe initiation, failure, dead zones and detonation simultaneously. The most important parameter is P1, the pressure between the initiation and failure regions. Both dead zone formation and failure can be largely controlled with this knob. However, V1 does failure with low settings and dead zones with higher settings, so that it cannot fulfill its purpose in the current format. To this end, V2 is under test. The derivation of the initiation threshold P0 is discussed. The derivation of the initiation pressure-tau curve as an output of Tarantula shows that the initiation package is sound. A desensitization package is also considered.

Terms:

A	code initiation compression, set to the fraction 0.1
AP	code A term in the JWL
B	code pressure exponent for a simple-JWL++ booster
B1	code pressure exponent for Tarantula initiation region
B2	code pressure exponent for Tarantula failure region
B3	code pressure exponent for Tarantula detonation region
BP	code B term in the JWL
C1	code power of (1-F) in the initiation region
C2	code power of (1-F) in the failure region
C3	code power of (1-F) in the detonation region
CP	code C term in the JWL
E0	code total detonation energy density in the JWL
F	burn mass fraction
Fde	desensitized mass fraction
G	rate constant for a simple-JWL++ booster
G1	code rate constant for Tarantula initiation region
G2	code rate constant for Tarantula failure region
G3	code rate constant for Tarantula detonation region
Gde	code rate constant for desensitization
KAPPAR	code kappa value of Murnahan unreacted EOS
NR	code n value of Murnahan unreacted EOS
P_o	measured initiation pressure threshold
P0	code pressure at initiation turn-on
P1	code pressure between initiation and failure
P2	code pressure between failure and detonation
POFF1	code pressure subtracted in the initiation region
POFF2	code pressure subtracted in the failure region
POFF3	code pressure subtracted in the detonation region
R1	code R1 exponent in the JWL
R2	code R2 exponent in the JWL
w	code omega exponent in the JWL

AR, QMULT, VR -ignore

1. Tarantula V1

Tarantula V1 (version 1) is an explosive kinetic package intended to do detonation, shock initiation, failure, corner-turning with dead zones, gap tests and air gaps in reactive flow hydrocode models with unchanged settings. The goal for Tarantula is to be initially calibrated, then used, and not changed for each experiment. We previously discussed details of V1 inside JWL++ as used on ambient LX-17 [1].

Tarantula V1 reacts sequentially toward detonation with the first four rate functions defined here, where P0, P1 and P2 mark the boundaries between the regions:

$$\text{P means Pressure} + \text{Artificial Viscosity}$$

$$\frac{dF}{dt} = 0, < \text{P0 NO REACTION} \tag{1}$$

$$\frac{dF}{dt} = G1(P - POFF1)^{B1}(1-F)^{C1}, \text{ P0 to P1 INITIATION} \tag{2}$$

$$\frac{dF}{dt} = G2(P - POFF2)^{B2}(1-F)^{C2}, \text{ P1 to P2 FAILURE} \tag{3}$$

$$\frac{dF}{dt} = G3(P - POFF3)^{B3}(1-F)^{C3}, \text{ P2 to P3 DETONATION} \tag{4}$$

$$\frac{d(Fde)}{dt} = -(Gde)P^{(Bde)}, \text{from 0 to Pde, Desensitization.} \tag{5}$$

Here, F is the burn fraction, t the time, P is the hydrocode pressure, which is the sum of real pressure and artificial viscosity. The use of artificial viscosity in the rate greatly helps with coarse zoning by adding additional pressure that keeps the rate constant low. With fine zoning, the influence of artificial viscosity should decrease. A first-order solver handles the discontinuities between the regions. The model is used here in an analytic functional form but point-by-point programming with linear interpolation is also possible.

P0, P1 and P2 mark the region boundaries listed in Eqs. 1 to 5. For ambient LX-17 In the initiation region, we always use

$$POFF1 = P0 = 0.075 \text{ Mb}; \quad C1 = 1. \tag{6}$$

In the failure region, we almost always use

$$POFF2 = 0 \text{ Mb}; \quad B2 = 0; \quad C2 = 1. \tag{7}$$

Now and then, we use a non-zero B2, which requires

$$\mathrm{POFF2} = \mathrm{P0} = 0.075\ \mathrm{Mb};\ \ \mathrm{C2} = 1. \tag{8}$$

In the detonation region, we use

$$\mathrm{POFF3} = 0\ \mathrm{Mb};\ \ \mathrm{B3} = 0;\ \ \mathrm{C3} = 1.5. \tag{9}$$

The use of the $(1\text{-F})^{3/2}$ was set up with Simple JWL++ to get a straight size effect line, and we are still using it.

From zero pressure to Pde, the desensitization rate comes on and removes LX-17 out of the path of being reacted, ie. it creates "unreactive LX-17" of mass fraction Fde. This mass fraction is can never contribute to the burn mass fraction, F. Because we know nothing about real desensitization, we use a constant rate, Gde, with a zero power of the pressure, Pde. Desensitization in LX-17 occurs before initiation occurs. This feature has no effect whatever on cylinder, ratesticks and most corner turning experiments.

The A, B, C "density" form of the JWL is used for accuracy. The "energy" form in effect lets the code pick the energy constant and this makes knowledge of the EOS uncertain. A Murnahan unreacted EOS is also used.

The parameter A turns on the reaction at some fraction of volume compression, and it historically been set at 0.1. The use of P0 puts another turn-on function in competition with A. If A is reduced, then G2 must be increased to get detonation. The results appear to be about the same.

The four pressure regions are shown in Figure 1. The red curve is the old simple quadratic rate used in Simple JWL++ and Linked CHEETAH. It turns on at zero pressure and steadily increases, so there is no way it can fail. The blue curve is Tarantula, where the four regions are very obvious. In Figure 1, the Y-axis is the reaction rate divided by the mass fraction term.

There are two thresholds in Figure 1. The P0 threshold shifts the start pressure for the P-τ initiation curve. The P1 and P2-jumps together form the second threshold, and this is what causes failure. Ignition and growth (I&G) has the P0 threshold, although it appears in terms of volume. However, I&G does not have the second threshold. By exchanging the regular P^2 rate to P^3, I&G is moved to the edge of model stability, and can fail, but the failure is numerical, not

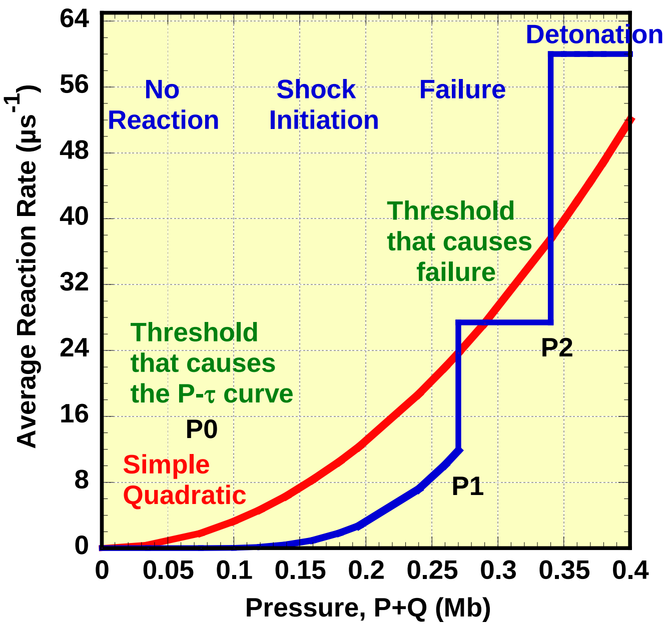


Figure 1. The one-reaction rate curve for simple quadratic and the four regions of Tarantula. Two thresholds are seen: initiation and failure.

physical. The pulsations of the model at this point further indicate that I&G is near the breaking point. It is necessary to introduce a real threshold cliff into the rate to get failure in a reproducible way. Two jumps are needed to currently calibrate the model, and a more couth descendent may be able to do this in one step.

Previously, we ran Tarantula on LX-17 in square zoning from 40 to 200 zones/cm using monotonic Q as the artificial viscosity. We had a complaint that results were directional in radial zoning and so we here also try out the bulk Q (qmodel3, qlin 0.25, qquad 2.0) as well. We use 40 square zones/cm as the coarsest mesh, although it is possible to force Tarantula down to 25-30 zones/cm. We next jump to 120 zones/cm, where the behavior starts to converge and end at 200 zones/cm.

2. Calibrating Dead Zones at 40 zones/cm

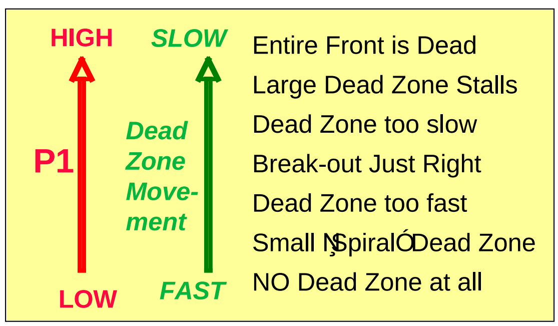
When calibrating Tarantula for dead zones and failure, the single knob that has the most effect is P1, the pressure between the initiation and failure regions.

1. If P1 is low, the dead zone is “fast”. The front is curved and can jump into the turn easily, so the detonation speeds around the corner quickly, possibly so fast that no dead is created at all.

2. If P1 is high, the dead zone is “slow”. The front is flat and the detonation speeds by the corner so fast it can’t turn. The dead zone forms but stops dead in its tracks, with no ability to turn the corner. At the worst, the entire front runs into a wide dead zone.

3. As P1 increases, failure turns on.

We may summarize the “dead-zone rule” with this P1 box:



For a double cylinder exercise, the LX-14 booster is set at b=2, G=1400. In every case, the 4 mm cylinder must show a detonation velocity between 7.33–7.35 mm/µs. Then, the 1-inch cylinder and the double cylinder with the steel end plate are run. The results, run with bulk Q, are shown in Figure 2. All points have P2 0.07 Mb higher than P1. The blue points have the proper 1-inch Cylinder detonation velocity of 7.54-7.56 mm/µs but the red points are too low.

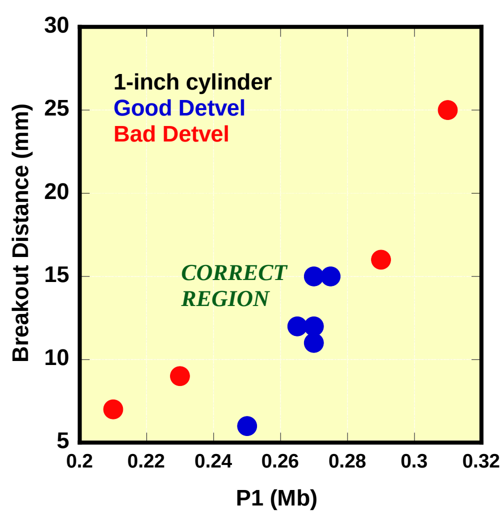


Figure 2. Double cylinder exercise to show that P1 is a knob to adjust the size of the dead zone.

Unfortunately, all boosters at 40 zones/cm will react faster than LX-17 and so are too-coarsely zoned. This means that special fiddling with the boosters is sometimes needed to make the various dead zone experiments work. This does not help the generality of the model but it can't be helped. For the double cylinder, the small cylinder is supposed to be long enough for nearly steady state, so that we may light it with a line detonation across the entire radius. This leaves the booster rate constant G (usually 1400 for LX-14) as the only variable. As shown in Figure 3, this can be used to center the distance in the desired area.

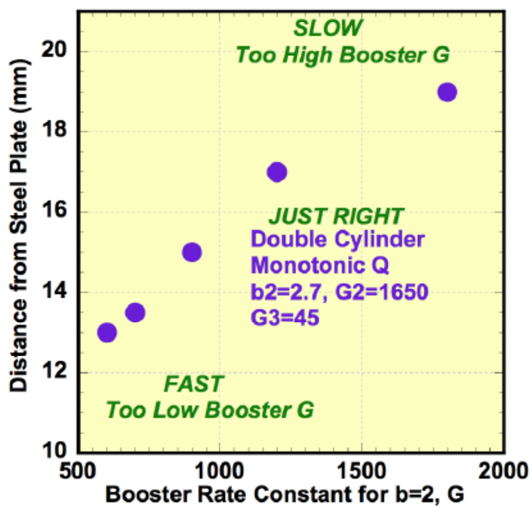


Figure 3. Double cylinder distance on edge from steel to first breakout as a function of the Simple JWL++ LX-14 booster rate constant.

The desensitization model is not needed and does not interfere with cylinders, air well or double cylinders. Its first use is shown in Figure 4, where we plot the aluminum plate velocities from Jack Rabbit3 [2]. In this experiment, a detonation must run around to the back-side of a steel plate, but a low shock back through the steel preceeds it. The LX-17 behind the steel is pre-compressed and this can affect the motion of the aluminum plate on the edge. In Figure 2c, we show the data taken by heterodyne velocimetry of an edge plate at 20 mm off-axis at 40 zones/cm. The model run with no desensitization, Gde = 0, has a velocity that is too high with Gde= 0.5 being about right. This was run with bulk Q and (1-F). The Gde setting will change with the parameters.

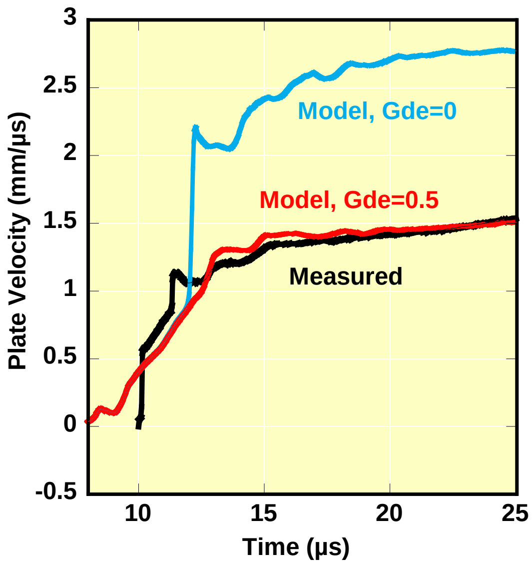


Figure 4. Effect of the desensitization parameter Gde on the plate velocities of Jack Rabbit3. A setting of 0.5 is about right. The heterodyne position at 20 mm on the aluminum edge plate is shown.

3. Run-to-Detonation Calibration at 40 zones/cm

We next turn to the initiation region of Tarantula. Luckily, this can be calibrated and fixed independently of the rest of the model. In the models, we use sabots long enough to hold up the pressure in the explosive at a constant level. The radius must be large enough that side rarifications have no effect. We use copper flyers, because the code and simple impedance calculations agree for this, whereas they do not for kapton. The results are listed in Table 1.

Table 1. Measured and calculated run-to-detonation times for various explosives in Mb units.

	LX-17		
P0	Ambient	0.075	0.075
B1	1.90	3.0	3.0
G1	g/cc	1600	1600
	measd	bulk	monot
initiation	**run-det**	Q	Q
pressure	**time**	40 z/	40 z/
(GPa)	**(µs)**	cm	cm
22.5	**0.2**	0.2	0.0
20.0	**0.35**	0.3	0.2
17.5	**0.6**	0.6	0.45
15.5	**0.9**	0.85	0.8
12.5	**1.75**	2.3	2.10
11.0	**4.5**	4.5	4.35
9.0			

We recall that the initiation region is described by the rate

$$\frac{dF}{dt} = G1(P - POFF1)^{B1}(1-F)^{C1}, \text{ P0 to P1 INITIATION,} \tag{2}$$

so that we end using B1 = 3.0, G1 = 1600 for both Q's at 40 zones/cm. One big advantage of our format is that the initiation region interacts weakly with the rest of the model, and once set, remains constant despite changes elsewhere.

A major parameter is the initiation threshold P0, and we now consider where this comes from. P0 is the infinite-pulse-length pressure for shock initiation. It is the lowest possible pressure that can ever cause initiation, and it works only for long pulses. The P0's were determined by combining several methods: run-to-detonation, flyer P-τ initiation and gap tests [3-13]. The results are shown in Figure 5 for pure ambient TATB and high-% TATB explosives. The fit through all the data is

$$P_O(\text{GPa}) \approx 1.0557e-5\exp(7.1895\rho_O). \tag{10}$$

It seemed that this might be usable at all temperatures if we use thermal expansion data to adjust the density. We have experimentally-obtained P0's for PBX 9502 of 10, 6 and 2 GPa at -55^{O}C, 75^{O}C and 250^{O}C, where the scatter is probably $\pm$1 GPa. Using Eq. 10 for the densities at each temperature, we get 10.7, 6.7 and 3.1 GPa at the three temperatures, and it appears that this process works within error.

In the Tarantula model, we use 0.075 Mb at 40 zones/cm for P+Q for ambient LX-17 even though Eq. 1 gives 0.090 Mb. We don't know enough about our model to explain why or whether it is really necessary, so we use at this time

$$P0(\text{Tarantula}) \approx 0.833P_o(\text{measured}) \tag{11}$$

for all.

With the combination of setting P0 and calibrating the run-to-detonation time (Pop plot) data, we next use Tarantula at 40 zones/cm to calculate the initiation threshold, which is shown in Figure 6. The ambient LX-17 initiation is from Honodel, et. al [14]. The error bars were derived by

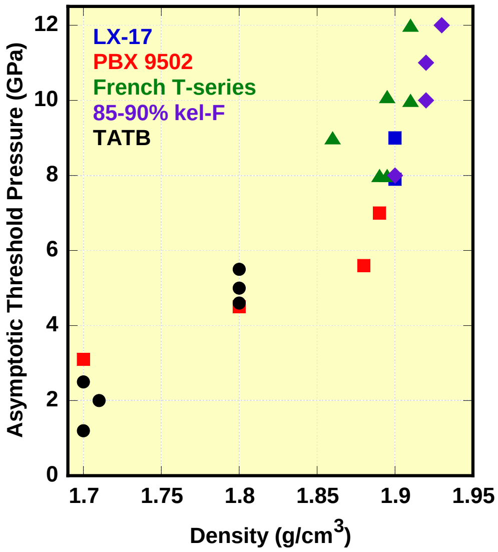


Figure 5. Measured P_0 for pure ambient TATB and >85% TATB mixtures.

C. Souers after going through the original data books found in the attic. The data was taken on small samples using the notch method to get velocities and aluminum silicofluoride to determine detonation. Our error bars are twice the flyer velocity error bars given in the paper.

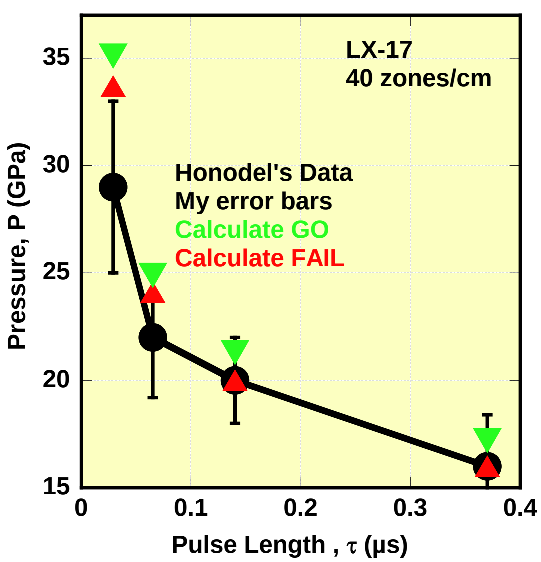


Figure 6. Calculated initiation threshold P-τ curve for ambient LX-17.

4. The Problem with Tarantula V1

The procedure for calibrating LX-17 with Tarantula V1 is shown in Figure 7. Implicit in this scheme is the assumption that all failures are the same and that one set of parameters will work for everything. Because Tarantula began as a dead zone model, dead zones get run before failure.

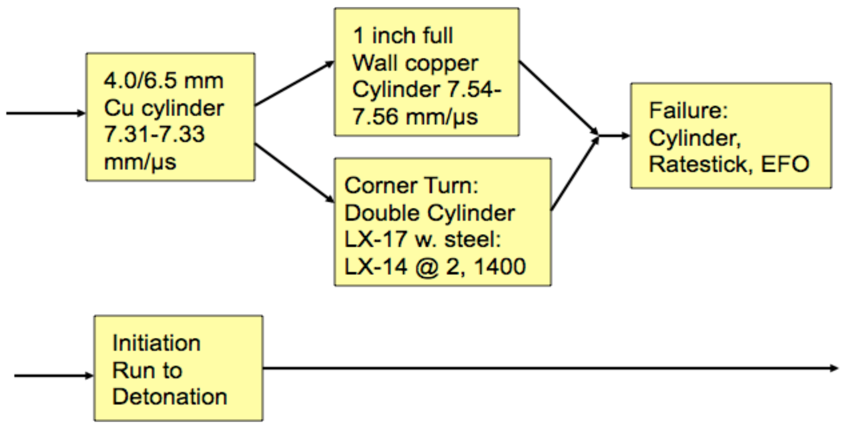


Figure 7. Tarantula calibration used for LX-17.

The results are summarized in Table 2. The dead zones are represented by the double cylinder with the steel back-up plate. Failure is given for the copper cylinder, the bare ratestick and the ratestick with an optical fiber (EFO) in it. Bulk and monotonic Q are used. The data roughly breaks into low and high branches, where low and high refer to P1. The low branch, which is what we have been generally using, works for the dead zones plus the 4 mm cylinder and the 7 mm rate stick, but not for 3 mm cylinder failure. The high branch is set to make the 3 mm cylinder fail, and the 4.5 mm ratestick fails along with it. Unfortunately, the 7 mm ratestick also fails and the 0.4-inch EFO is on the edge. We may say roughly that the low branch seems to represent lower shocks, as are seen in the corner-turn. The high branch represents higher shocks in the prompt detonation regime. This degree of detail appears to be real and is not represented in the model as it stands.

To summarize: Tarantula V1 assumes that the rates switch at certain constant pressures. From gauge initiation data, we believe that this is not true: that the switching points are a function of initiation pressure. A version of Tarantula V2 has been designed, and it is being tested at this time. V2 is designed to bring dead zones and failure together.

Table 2. Tarantula V1 results for ambient LX-17, showing the split into a low and a high branch.

Po=0.075 Mb all				P1	dead	7.0 mm	0.4 inch	4.5 mm	3 mm
zones/	type	Q	A	(Mb)	zones?	ratestick	EFO	ratestick	cylinder
cm						run 7.40	FAIL	FAIL	FAIL
40	Low	bulk	0.1	0.27	yes	runs	runs	runs	runs
40	Low	bulk	0.026	0.27	yes	runs	runs	runs	runs
40	Low	monot.	0.1	0.26	yes	FAIL	FAIL	FAIL	FAIL
120	Low	bulk	0.1	0.18	yes	runs	runs	runs	runs
120	Low	monot.	0.1	0.18	yes	runs	runs	runs	runs
200	Low	bulk	0.1	0.18	yes	runs	FAIL	runs	runs
40	High	bulk	0.1	0.365		FAIL		FAIL	FAIL
120	High	bulk	0.1	0.25	no	FAIL	1-inch fail	FAIL	FAIL
120	High	bulk	0.1	0.25	no	FAIL	1-inch fail	FAIL	FAIL
120	High	monot.	0.1	0.25	no	FAIL	1-inch fail	FAIL	FAIL
200	High	bulk	0.1	0.25	no	FAIL		FAIL	FAIL

Po=0.075 Mb all	P1	P2					
zones/	Q	(Mb)	(Mb)	b1	G1	b2	G2	G3
cm								
40	bulk	0.27	0.34	3.0	1600	0	27.4	60
40	bulk	0.27	0.34	3.0	1600	0	60	60
40	monot.	0.26	0.32	3.0	1600	0	25	60
120	bulk	0.18	0.32	1.0	4	0	21	55
120	monot.	0.18	0.32	1.0	4	0	22	55
200	bulk	0.18	0.32	1.0	4	0	21	55
40	bilk	0.365	0.425	3.0	1600	0	47.4	60
120	bulk	0.25	0.32	1.0	4	0	25	55
120	bulk	0.25	0.32	1.0	4	0.5	55	55
120	monot.	0.25	0.32	1.0	4	0	24	55
200	bulk	0.25	0.32	1.0	4	0	25	55

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Acknowledgments

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